

2,3-Dibromothiophene
3140-93-0 | DTXSID80185324

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.85 | 0.69 | 0.86 | 0.67 | 0.86 | 0.78 |

Model Results

Predicted value: 3.53

Global applicability domain: Outside

Local applicability domain index: 4.34e-01

Confidence level: 7.13e-01

Nearest Neighbors from the Training Set

| | | |
|--|---|---|
| <div>Image not found</div> <div>Pentachloroethane</div> <div>Measured: 3.22</div> <div>Predicted: 3.19</div> | <div>Image not found</div> <div>Tetrachloroethylene</div> <div>Measured: 3.40</div> <div>Predicted: 3.35</div> | <div>Image not found</div> <div>Hexachloroethane</div> <div>Measured: 4.14</div> <div>Predicted: 4.00</div> |
| <div>Image not found</div> <div>3H-1,2-Dithiole-3-thione, 4-methyl-</div> <div>Measured: 2.18</div> <div>Predicted: 2.20</div> | <div>Image not found</div> <div>Hexachloro-1,3-butadiene</div> <div>Measured: 4.78</div> <div>Predicted: 4.65</div> | |